Direct structure determination of epitaxially grown films.

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Introduction.

Epitaxially grown films are physically exciting because their properties are often substantially different from the properties of the bulk materials and are important because they play a very important role in various microelectronic and optoelectronic devices. Determination of their atomic structure in particular close to the film substrate interface is essential for the understanding of their properties. During the past few years we have developed a new direct method[1], based on Coherent Bragg Rod Analysis COBRA, to determine their structure. During the last year the method has been brought to fruition and applied to two systems: Gd_2O_3 grown on (1 0 0) GaAs and $BaTiO_3$ grown on (1 0 0) $SrTiO_3$.

The structure of Gd_2O_3 grown on (1 0 0) GaAs.

Gd_2O_3 has been shown to be a very effective passivation layer for GaAs allowing the formation of high quality field effect transistors in GaAs[2]. To determine the atomic structure of these films we measured their x-ray diffraction along 13 symmetry inequivalent substrate defined Bragg rods. We then used COBRA to determine the complex scattering factors along the Bragg rods and Fourier transformed the scattering factors into real space to obtain the electron density and structure of the system.

The results confirm the finding of Kortan et al. [3] that the film is a single domain and show in addition that the film substrate interface and the film surface have transition regions of about 5 Gd_2O_3 layers resulting probably from interface and surface roughness. The results reveal two rather surprising features:

First, the stacking order of the layers in the film is different from the stacking order of the corresponding layers in bulk Gd_2O_3. In both Gd_2O_3 and GaAs the structure repeats itself every 4 layers. In Fig. 1 we show the in-plane Gd positions in 4 consecutive Gd_2O_3 layers together with the positions of Ga and As in 4 consecutive layers of the GaAs substrate. Notice that the relative positions of the Gd and Ga/As atoms remain approximately the same in all 4 layers.

Second, The COBRA determined electron density shows that the Gd atoms in the first 3 Gd_2O_3 layers in rows 1,2,4 and 5 are displaced so that they overlap exactly the in-plane Ga/As positions. As the distance from the interface increases the positions relax to the positions expected from bulk Gd_2O_3.

The way the Gd_2O_3 conforms to the GaAs structure may be at the bottom of the fact that this material forms an excellent passivation layer for GaAs.

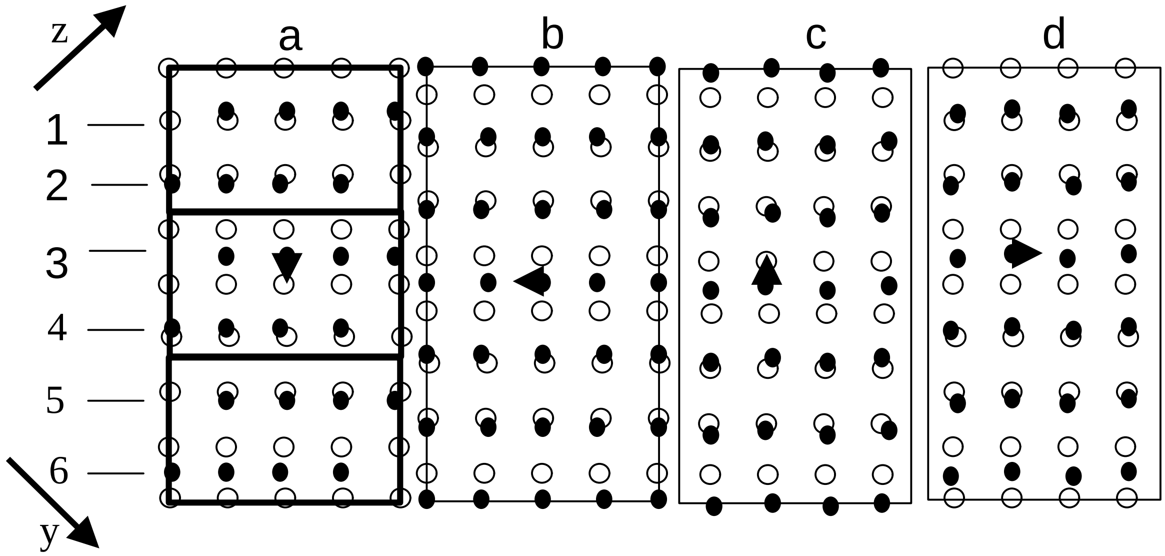

Fig. 1. Gd positions in 4 consecutive layers shown as dots. Notice that the positions in one layer can be approximately obtained from the positions in the previous layer by shifting them by the vector shown in that layer. (The last vector on the right shifts the positions from the last layer to the first). The circles represent Ga and As positions in 4 consecutive layers of GaAs.

The structure of $BaTiO_3$ grown on (1 0 0) $SrTiO_3$.

$SrTiO_3$ is an incipient ferroelectric while $BaTiO_3$ is ferroelectric at room temperature. We have investigated the structure of epitaxially grown BaTiO3 on (1 0 0) $SrTiO_3$. The diffraction intensities were measured along the $SrTiO_3$ defined Bragg rods. Then, using COBRA we obtained the complex scattering factors along the Bragg rods and Fourier transforming them yielded the three dimensional electron density and atomic structure of the system. The results show that the vertical Ba-Ba distances are larger than in Bulk $BaTiO_3$ but otherwise almost all atoms are in centro-symmetric positions within the experimental accuracy of 0.1 A. The exceptions are the oxygen atoms in the Sr and Ba planes parallel to the interface. Close to the interface on both $SrTiO_3$ and $BaTiO_3$ sides the O atoms in the Sr and Ba planes are displaced by upto 0.3 A. These displacements are shown in Fig. 2 as a function of layer No.

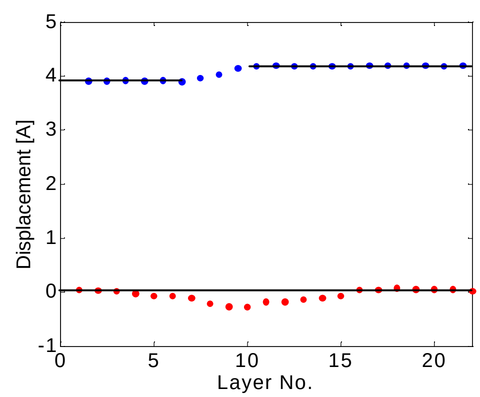

Fig. 2. Sr-Sr distances (left) and Ba-Ba distances (right) -blue dots. Vertical displacements of O atoms in the Sr and Ba Planes - red dots. The lines are guide to the eye.

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